Improvements to the Finite-Temperature Average-Atom Model

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Radiative properties of hot, dense plasmas remain a subject of current interest. In many plasma environments, the effects of the free electrons on the bound electrons cannot be neglected. The principal approach used previously for the inclusion of such effects is termed the average-atom (AA) model. In this approach, the Kohn-Sham equation is solved for the bound electrons in several possible approximations to model the response of these electrons to the plasma environment.

Recently a program of work has been underway to describe the response properties of atoms (or ions) in hot, dense plasmas, using what is known as the Finite-Temperature Random-Phase-Approximation (FTRPA) in the calculation of spectral properties of the plasma. This was first introduced by des Cloizeaux [1]. This approach produces the appropriate potential for the calculation of the wavefunctions of the excited electrons. This work was greatly extended and developed by Csanak and Kilcrease [2], who derived expressions from which the linear response function can be calculated, which allows a straightforward calculation of spectral quantities such as the photoabsorption cross section and the oscillator strength. More recently, this approach has been further developed by Csanak and Meneses [3] to formulate the FTRPA approach into a tractable system of coupled integro-differential equations. These equations were then solved by Csanak and Meneses [3], and Csanak and Daughton [4] in the uncoupled "single-channel" approximation for hot helium and lithium plasmas at a variety of densities.

The current work on this subject has focused on solving the full set of coupled FTRPA integro-differential equations. The solution of these equations is based on the Linear Algebra method [5], which is a well-known, robust, numerical technique for the efficient solution of coupled equations. This technique has previously been used with considerable success in electron-molecule scattering [6]. We chose to focus on the spectroscopic properties of neon-like ions in finite-temperature systems, in which coupling effects should be more pronounced than in helium-like or lithium-like systems.

As a check on our method, we first solved the FTRPA coupled-channel equations at zero temperature and density in order to compare with previous results from atomic physics calculations. At finite temperature and density, there are no previous results with which to compare. Figure 1 shows the oscillator strength for a selection of neon-like ions calculated in various approximations. In (a) we show the oscillator strength calculated in the single-channel approximation formulated previously [3, 4] and we compare with configuration-average calculations from the well-established atomic structure code, CATS, developed at Los Alamos by Cowan and coworkers [7]. It is clear that the two methods are in excellent agreement. In (b) we present the oscillator strength calculated using our current coupled-channel approach. Again, we compare with calculations from the CATS code, which in this case is run in the fine-structure approximation, which includes configuration-interaction effects in a manner that is similar, but not identical, to the coupled-channel approach of the FTRPA equations. In this case we see good agreement between the two sets of calculations over a wide range of ion charges. The coupling between the channels has increased the oscillator strength by well over 20%, even for high Z.

We are currently applying the solution of the coupled-channel FTRPA equations for neon-like systems at finite temperatures and densities. In this case, we use the average-atom model developed by Daughton and Snell [8], which includes a "pseudo-atom" approach for the interaction of the "average-atom" with the rest of the plasma. This allows the energy of the system to be clearly defined, so that the resulting equation-of-state is unambiguous. We hope to report these new results in the near future.

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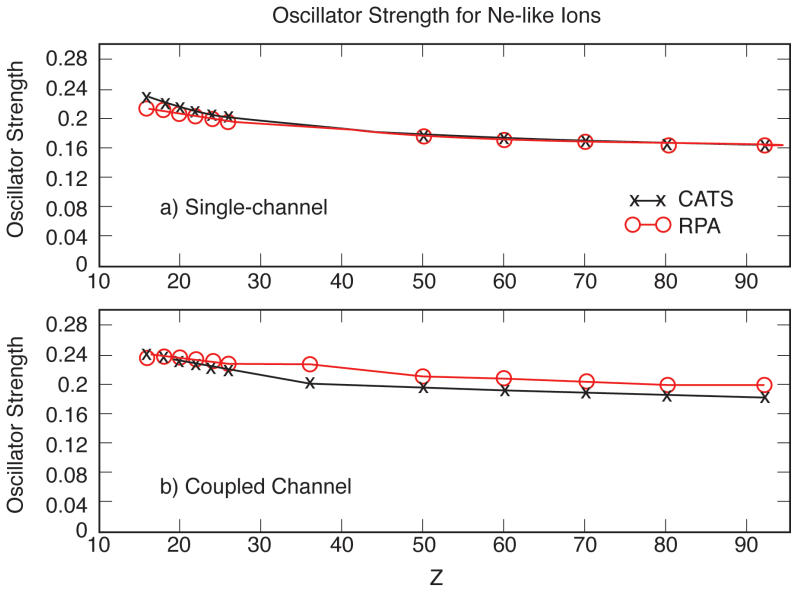

Fig. 1.
Oscillator strength for a selection of neon-like ions calculated in various approximations. (a) Oscillator strength calculated in the single-channel approximation formulated previously [3, 4] compared with configuration-average calculations from CATS; and (b) the oscillator strength calculated using our current coupled-channel approach compared with calculations from the CATS code, which in this case is run in the fine-structure approximation, including configuration-interaction effects in a manner that is similar, but not identical, to the coupled-channel approach of the FTRPA equations.